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# Spin-triplet and spin-singlet superconductivity in the Hubbard model on a triangular lattice

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**Abstract**

Within third-order perturbation theory, we discuss the possibility of spin-triplet and spin-singlet superconductivities in a two-dimensional Hubbard model on a triangular lattice for some model parameters corresponding to the heavy-fermion superconductors $UM_2Al_3$ (M = Pd, Ni) and organic superconductors under uniaxial strain. In the model of the heavy-fermion superconductors $UM_2Al_3$ (M = Pd, Ni), when we vary the symmetry in the dispersion of the bare energy band from $D_2$ to $D_6$, spin-singlet superconductivity in the $D_2$-symmetric system is suppressed and we obtain spin-triplet superconductivity in the nearly $D_6$-symmetric system. We point out the possibility that the results obtained correspond to the difference between the superconductivity of $UPd_2Al_3$ and that of $UNi_2Al_3$. In the model of organic superconductors under uniaxial strain, when we increase the diagonal hopping integral to above 1.2, we obtain the tendency for spin-triplet superconductivity to emerge. In all cases mentioned above, it is found that the vertex correction terms, which are not included in the interaction mediated by the spin fluctuation, are essential for realizing the spin-triplet pairing.

## 1. Introduction

We discuss the superconductivity in a two-dimensional Hubbard model on a triangular lattice for some model parameters corresponding to two situations mentioned below. First, we consider the isostructual hexagonal $PrNi_2Al_3$-type heavy-fermion compounds $UM_2Al_3$ (M = Pd, Ni). $UM_2Al_3$ (M = Pd, Ni) were found to be superconductors with $T_c \simeq 2$ and 1 K, respectively. Their superconducting states coexist with antiferromagnetic long-range orders with $T_N = 14.3$ and 4.5 K, respectively. The magnetism and superconductivity properties are different for the two compounds. $UPd_2Al_3$ orders in an antiferromagnetic long-range structure with a commensurate wavevector $\boldsymbol{k} = (0, 0, 0.5)$ and has a large ordered magnetic moment $\mu = 0.85\ \mu_B$ on uranium atoms. $UNi_2Al_3$ orders in a spin-density

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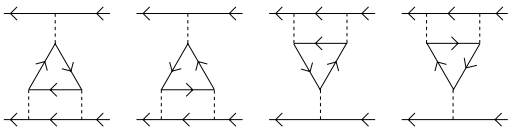

**Figure 1.** The solid and dashed lines correspond to the bare Green function and the interaction, respectively.

wave (SDW) with an incommensurate wavevector $\boldsymbol{k} = (H \pm 0.61, 0, 0.5)$ and has a tiny magnetic moment of 0.2 $\mu_B$ whose magnitude is modulated within the basal plane. As regards the superconducting properties, various experiments suggest that $UPd_2Al_3$ is a spin-singlet d-wave superconductor with a line-node gap. On the other hand, spin-triplet superconductivity in $UNi_2Al_3$ has been revealed by NMR measurement recently [1]. We attempt to explain the difference between the superconductivity of $UNi_2Al_3$ and that of $UPd_2Al_3$ from the viewpoint of the differences in symmetry (fermiology) in the itinerant electron systems with different antiferromagnetic structures. Next, we consider organic superconductors under uniaxial strain. Recently, Maesato *et al* [2] developed a uniaxial strain method for artificially controlling the electronic properties of organic conductors by reducing the intermolecular distance along a desired direction without changing those along other directions. On the basis of the assumption that electron correlation induces the superconductivity in organic superconductors, we investigate the possibility of both spin-triplet and spin-singlet superconductivity in organic superconductors under uniaxial strain without assuming a spin-fluctuation-mediated mechanism, as had been done by Nomura and Yamada in investigating the mechanism of superconductivity in $Sr_2RuO_4$ [3]. Spin-fluctuation-mediated spin-triplet superconductivity has been investigated by Kuroki and Arita in a similar model [4].

We adopt the following Hubbard Hamiltonian:

$$H = \sum_{\boldsymbol{k},\sigma} (\epsilon(\boldsymbol{k}) - \mu) a^{\dagger}_{\boldsymbol{k}\sigma} a_{\boldsymbol{k}\sigma} + \frac{U}{2N} \sum_{\sigma \neq \sigma'} \sum_{\boldsymbol{k}_1 \boldsymbol{k}_2 \boldsymbol{k}_3 \boldsymbol{k}_4} \delta_{\boldsymbol{k}_1 + \boldsymbol{k}_2, \boldsymbol{k}_3 + \boldsymbol{k}_4} a^{\dagger}_{\boldsymbol{k}_1\sigma} a^{\dagger}_{\boldsymbol{k}_2\sigma'} a_{\boldsymbol{k}_3\sigma'} a_{\boldsymbol{k}_4\sigma},$$

where $\mu$, $U$, and $\epsilon(\boldsymbol{k})$ are the chemical potential, the Coulomb repulsion, and the dispersion of the bare energy band on the two-dimensional triangular lattice, respectively. Our model parameters are the dispersion $\epsilon(\boldsymbol{k})$ of the bare energy band on a two-dimensional triangular lattice, the electron number $n$ per spin site, and the Coulomb repulsion $U$. We set up these model parameters for the situations mentioned above. We calculate the superconducting transition temperature $T_c$ by solving the Éliashberg equation. We expand the normal self-energy effective interaction with respect to $U$ up to third order. In the diagrams for the effective interaction up to third order, the vertex correction terms which are not direct contributions from spin fluctuations are included. The other diagrams are included in the RPA and fluctuation exchange (FLEX). In the case of spin-triplet pairing, we give the vertex correction terms included in the diagrams up to third order, in figure 1.

## 2. The heavy-fermion superconductors $UM_2Al_3$ (M = Ni, Pd)

$UM_2Al_3$ (M = Pd, Ni) undergo superconducting transitions below the Néel temperature. Therefore, the symmetry in the itinerant electron system with antiferromagnetic structure is one of the important matters to consider in investigating the mechanism of superconductivity. According to band structure calculations [5], the symmetry in the itinerant electron system of $UPd_2Al_3$ is not of hexagonal symmetry, reflecting the effect of the antiferromagnetic structure with a large ordered magnetic moment $\mu = 0.85\ \mu_B$ on the uranium atoms, and we have

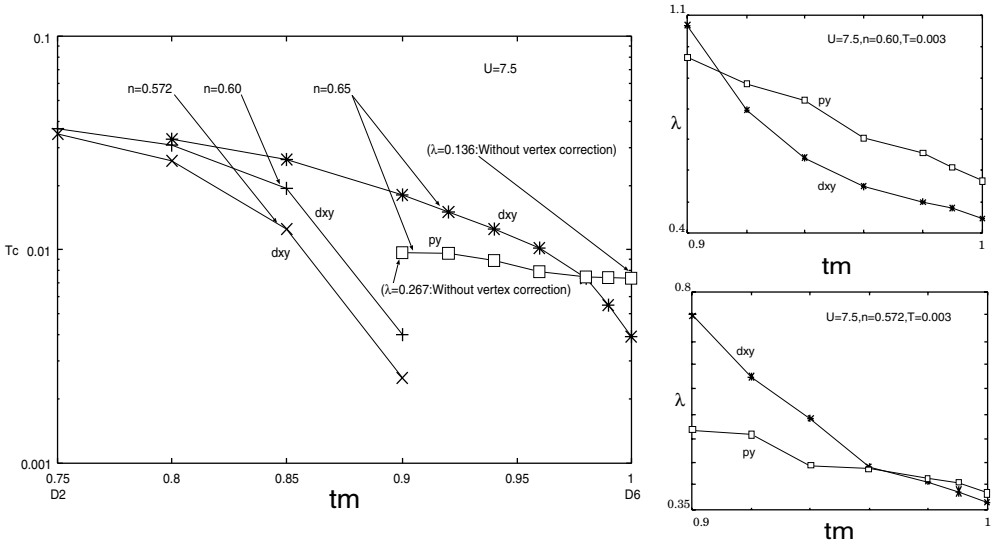


**Figure 2.** The calculated $T_c$-values (eigenvalues $\lambda$ of the Éliashberg equation) are shown as a function of $t_m$ for various $n$-values. In this figure, '($\lambda = \cdots$: Without vertex correction)' means that the eigenvalue $\lambda$ calculated without vertex correction terms is $\lambda = \cdots$ at $T_c$ obtained by using the third order perturbation theory.

treated this by considering the following dispersion of the bare energy band with the anisotropic hopping integral $t_m \neq 1$: $\epsilon(\boldsymbol{k}, t_m) = -4\cos(\frac{\sqrt{3}}{2}k_x)\cos(\frac{1}{2}k_y) - 2t_m\cos(k_y)$ [6]. We calculate here $T_c$-values (eigenvalues of the Éliashberg equation) for various values of $t_m$ and $n$, starting from the model parameters for $UPd_2Al_3$ ($t_m = 0.75, n = 0.572$). The results are shown in figure 2. In the case of $n = 0.572$ and $t_m = 0.75$, the spin-singlet state ($d_{xy}$) is the most stable. When we vary $t_m$ (the symmetry in the system) from $t_m = 0.75$ ($D_2$) to $t_m = 1$ ($D_6$), at the same time, the anisotropic nature of the spin fluctuation is suppressed. In this case, the spin-singlet state ($d_{xy}$) is suppressed because the main origin of the d-wave superconductivity is spin fluctuations, and we can see that spin-triplet states ($p_y$) emerge. In this case, we can see that it is found that the vertex correction terms are essential for realizing the spin-triplet pairing. In the context mentioned above, the symmetry in the itinerant electron system of $UNi_2Al_3$ may be more isotropic than the symmetry in that of $UPd_2Al_3$, because it reflects an incommensurate SDW order with a tiny moment of 0.2 $\mu_B$, although the detailed electronic structure of $UNi_2Al_3$ has not been investigated yet. Therefore, we assume that $t_m \simeq 1$ in the case of $UNi_2Al_3$. On the basis of the hypothesis mentioned above, our results seem to explain not only the mechanism of spin-triplet superconductivity in $UNi_2Al_3$ but also the difference between the superconductivity of $UNi_2Al_3$ and that of $UPd_2Al_3$, because the spin-singlet superconductivity in the $D_2$-symmetric system ($t_m \neq 1$) is suppressed toward $D_6$ symmetry, and the spin-triplet superconductivity emerges in the nearly $D_6$-symmetric system ($t_m \simeq 1$). In conclusion, we point out the possibility that the results obtained correspond to the difference between the superconductivity of $UNi_2Al_3$ and that of $UPd_2Al_3$.

## 3. Organic superconductors under uniaxial strain

We adopt here the following dimer model: $\epsilon(\boldsymbol{k}, t_1) = -2[\cos k_x + \cos k_y + t_1\cos(k_x + k_y)]$. The uniaxial strain method artificially changes the electronic properties of organic conductors by

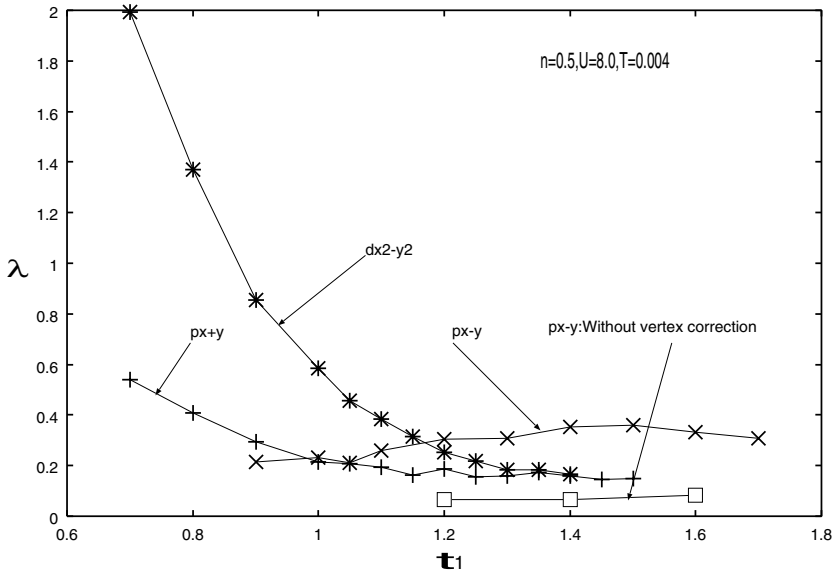


**Figure 3.** The eigenvalues $\lambda$ of the Eliashberg equation for various $t_1$-values at $n = 0.5$, $U = 8$, $T_{\rm lim} = 0.004$. $T_{\rm lim}$ is the lower limit temperature for reliability of our numerical calculation.

reducing the intermolecular distance along a desired direction without changing those along other directions. Therefore, it is considered that the uniaxial strain method is represented by changing $t_1$ (the diagonal hopping integral) in the dimer model. For example, the electronic states for $t_1 \geqslant 1$ can be obtained by using the uniaxial strain method. We calculate here the eigenvalues of the Éliashberg equation for various $t_1$ (0.9–1.7) at $n = 0.5, U = 8, T_{\rm lim} = 0.004$. The results are shown in figure 3. When we vary $t_1$ from $t_1 = 0.9$ to 1.7, the spin-singlet ($d_{x^2-y^2}$) state originating from spin fluctuations [7] is suppressed and we can see that spin-triplet states ($p_{x-y}$) have a tendency to emerge. In this case, we can see that it is found that the vertex correction terms are essential for realizing the spin-triplet pairing. In conclusion, we have obtained the tendency of emergence of spin-triplet superconductivity in the region $t_1 \geqslant 1.2$, based on the assumption that the superconductivities in organic superconductor under uniaxial pressure are induced by the electron correlation. But in the region $t_1 \geqslant 1.2$, the superconducting transition temperatures are expected to be too low. Therefore, another mechanism may become dominant for the superconductivities in real systems.

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